

CapSim 3.5 Quick- Start Manual

CapSim is designed to simulate contaminant transport in sediments. It was primarily developed to model contaminant transport through sediment caps for the purposes of design but it can also be used to simulate contaminant migration in uncapped sediments (e.g. for the evaluation of natural recovery) and in-situ treatment of sediments. The model is built on a foundation of sediment and cap modeling dating back to 1991 [1] and early versions were described in EPA guidance for capping in 1998 [2]. The current version is an extremely robust tool that includes capabilities for modeling contaminant transport in sediments under a wide range of conditions including

- Dynamics of multiple species with linked reactions in sediments, conventional and amended cap materials and sediment amendments
- Multiple layers of materials with widely varying physical and chemical conditions and material mixtures
- Diffusion/dispersion
- Bioturbation transport of contaminants modeled by both uniform mixing over depth or depth dependent bioturbation
- Bioturbation mixing of solids (e.g. to model sorbent intermixing into surficial sediments over time)
- Groundwater upwelling and tidal or oscillating flows with both time dependent and average fluxes or concentrations over oscillating flow cycles
- Sediment consolidation with input of characteristic time and 90% consolidation depth
- Sediment deposition and intermixing of deposition layer by bioturbation
- Linear and nonlinear sorption
- Equilibrium or non-equilibrium sorption
- Exchange at the sediment-water interface
- Estimation of water column concentrations for a finite well-mixed waterbody

CapSim is largely menu-driven and user can select options as needed. The model can estimate a variety of common sediment parameters or the user can override these estimates with their own inputs. The purpose of this guide is to introduce CapSim and how to use the program.

CapSim Installation

First, go to the website <http://www.depts.ttu.edu/ceweb/groups/reiblesgroup/> download the newest edition **CapSim Exe File** and set up the software. The program is available from “downloads” from the home page. You will be asked to input a password (“sediment”). Please send me a short note at danny.reible@ttu.edu so that we can add you to the list of users to notify you of any future updates.

After downloading, you can launch the self-installing file and install the program. Make sure that you are using the version of CapSim appropriate for your computer (either a 32 bit or 64 bit windows operating system version). You can also download this quickstart manual and databases of chemical information.

Main Menu

Upon starting the program, you will be presented with a main menu which are series of push button boxes which have the following options

- Create or load input file— CapSim uses an input file that saves all of your simulation options. There is a sample input file available (described below)
- Load existing results – if you have a previous executed simulation you can load the exported data file and examine plots from that simulation or compare multiple simulations on one plot
- Run a batch file – this is an advanced option to allow you to run multiple simulations without intervention. Two types of batch files are available, “Separate” and “Continuous”, and examples of both are included with the program. A “Separate” batch file allows running multiple configurations of the program just as if you running them one at a time and saving the results. The “Continuous” batch file allows you to stop a simulation at a given time and then pick it up with a different set of conditions or parameters due to system changes. An example might be deposition for a period of time followed by no further deposition.
- Edit chemical/material databases – these are the databases that provide CapSim basic data for the simulations. You can use a partially populated sample database or add your own information. You can also bypass the database and put information on materials and chemicals directly into a simulation as well. The database allows the information to be available to any simulation.

If you can't find the corresponding properties for the chemicals, sediments or the auxiliary conditions in the existing database or prefer to use your own data, you may want to edit the chemical database or material database first before you create the input file. For chemical properties, you may at least need molecular weight, Kow (octanol-water partition coefficient), Dw (molecular diffusion coefficient), Koc (organic carbon partition coefficient) and Kdoc (dissolved organic carbon partition coefficient) under the same temperature. You can have data at multiple temperatures for a single contaminant if desired. These parameters can be estimated by CapSim from Kow for hydrophobic organic compounds such as PAHs or PCBs. For metals, the Kow, Koc and Kdoc are not relevant and you might leave these blank and simply specify a partition coefficient, Kd, during the simulation. For material properties, porosity, bulk density, and organic carbon fraction are needed and you can choose the form of sorption model you would like to use for that material (constant Kd, Kocfoc (for organics), Langmuir or Freundlich). You have the option of changing these for a particular simulation but the database contains default values.

If you have a database from an old version of CapSim on your computer, you may need to delete that file before installing CapSim to avoid any complications with incompatibility.

CapSim Parameters

Most of the CapSim parameters are self-explanatory and follow standard usage. Some important parameters and their definitions within the program are summarized below

- Concentration – refers to truly dissolved porewater concentration (or potentially a total porewater concentration if your input concentrations under auxiliary conditions are total porewater concentrations)
- Bulk density – solid phase density of porous medium on dry basis, i.e. dry solid mass/total volume
- Sorption kinetics – modeled as a first order rate constant times the porewater concentration except for Langmuir sorption which has a rate model explicit in its formulation. For strongly sorbing contaminants, many porewater half-lives may be required to near equilibrium

- Velocity – is a Darcy velocity based upon total area and not just the void area. If U is the Darcy velocity and v is the seepage velocity based upon void area, ϕ , $U=v\phi$.
- Diffusivity – molecular diffusion coefficient in water. This is corrected for porosity and tortuosity of the medium within the program.
- Hydrodynamic dispersivity – dispersion is modeled as αU where α is the dispersivity (units of length) and U is the Darcy velocity
- Reaction kinetics – normal reactions are modeled as occurring in the porewater only and the overall first order reaction rate per unit total volume, k_{vol} , is then related to the input reaction rate, k , by $k_{vol}=k\phi$ where ϕ is the porosity or void fraction of the medium.

A Simple CapSim Simulation Example

After you finish the database modification part, you can click on "Create new input file" or "Input existing input file" to set up a particular simulation. If you selected create a new file or input existing results you will first be faced with a window for selection of units in which you would like to work. Click on one of the push buttons and available options can be selected.

Going over a simple example will give you a better understanding of what data you need and what output is expected. Click on "Load existing input file" and open "input_example.cpsm". A summary of the example simulation will appear with push button boxes on the right hand side of the screen. You may need to expand the box or move the slider up or down on the right hand side to see all of the simulation inputs.

Contaminants and Properties

The contaminants in the sediment in this example are phenanthrene, mercury and methylmercury. The reactions included are methylation, demethylation and phenanthrene decay. Here, we assume they are all first order reactions. Note that the methylation and demethylation reactions are coupled and formation of methyl mercury reduces total mercury and vice versa. To edit chemical properties click on either the first option box on the right or the second to modify reactions. To edit properties or reactions, you can click the word edit on the far left of the resulting pop up window (or delete to remove the line entirely). When entering values, make sure you pay attention to the units requested.

Materials and Layers

The example system contains three layers, namely, 10.0 cm of sand, 2.0cm of activated carbon and 10.0 m of sediment from top to bottom. There is also a layer for depositing sediment (in the length and time units- in this case 0.1 cm per year). Typically you would use at least one sediment layer and, if simulating a cap, a layer for each layer of a cap. You can also eliminate the sediment layer if you wish to model the sediment as a constant concentration boundary. It is normally better to model the sediment explicitly, however, because there is typically depletion over time in the contaminated sediment. You can model multiple sediment layers if you have measured concentration profiles as a function of depth. You would then specify the initial concentration in each layer from the known depth profile (see auxiliary conditions below).

Layers are defined by first selecting the materials to be used from the materials database or by adding a new component to a mixture. If an existing material (load component) you can select the material by pushing the name button and selecting the appropriate component and then entering the weight fraction of that component in the mixture. The physical properties of the selected component will be

automatically loaded. If you are adding a new component you should enter the material properties including porosity, bulk density and organic carbon content of the component. This information is used to estimate the mixture properties assuming an ideal mixture of the components (that is, the total volume is the sum of the volume of the individual components- this may not be true for mixtures of substantially different particle sizes and in such cases you should calculate or measure the mixture characteristics separately and define it as a new material for capsim).

In previous versions of CapSim, the volume fractions were entered. The total mass of the component (e.g. AC) in the mixture is calculated differently for volume fractions or weight fractions and this should be considered when considering how much of a component to add.

CapSim v3.3 or before – volume fractions entered

Mass/area of mixture component = (volume fraction) \times (bulk density of *component*) \times (layer thickness)

CapSim v.3.4 – mass fractions entered

Mass/area of mixture component = (weight fraction) \times (bulk density of *mixture*) \times (layer thickness)

In particular, setting the mass fraction means that changing the bulk density of a particular component will primarily change the volume needed to be added to the layer to achieve that weight fraction. When setting the volume fraction, you could directly change the mass of the component by changing the bulk density of the component. For example, if you wanted to reduce the amount of activated carbon in a mixture with an inert material, in older versions of CapSim you could simply reduce the bulk density of the activated carbon while maintaining the volume fraction. In the current version, this may have minimal impact on the bulk density of the mixture and therefore would only change the volume of activated carbon needed to be added to achieve the desired weight fraction. **When unsure about how much of a mixture component is being added, you should calculate the mass per unit area being added with the equations above.**

As an example consider a 50:50 mixture of sand (bulk density of 1.25 g/cm³) and Aquagate containing 10% activated carbon (bulk density of mixture 1.09 g/cm³ from 90% aggregate of 1.35 g/cm³ and 10% activated carbon, 0.4 g/cm³). You have two options

1. Input the mixture as being 50% sand, 45% aggregate and 5% AC with their respective pure component bulk densities and sorption properties.
2. Input the mixture as being 50% sand and 50% Aquagate with the Aquagate density being 1.09 g/cm³. In this case you must specify the sorption in this layer as though it is 10% of the sorption of a pure activated carbon layer. For example, specify the K_f in the Freundlich isotherm to be 10% of pure activated carbon.

Note that if you want to have layers of the same material with different physical properties (e.g. a depositing sediment layer that has a porosity of 0.8 and a consolidated sediment layer that has a porosity of 0.5) you should define the two different sediment types in the solids database and give them names that you can use to distinguish between them (e.g. surface sediment and consolidated sediment).

If you change the material properties or add materials, the sorption pop up box will automatically appear allowing you to change both the type and parameter values for sorption in each material. Sorption

relationships that can be used include a specified linear partition coefficient, the classic model of a partition coefficient as the product of the fraction organic carbon and the organic carbon based partition coefficient, a Langmuir isotherm and a power law Freundlich isotherm. Database files are available that have sorption data on a variety of organic contaminants. Local equilibrium or transient sorption kinetics can also be assumed. Transient sorption is assumed to follow first order kinetics if chosen. If you want to modify any of the default or database properties, you can click on the sorption properties or layer properties to edit either.

Layers are laid out top to bottom using the materials that you have defined. The thickness of the layers, dispersivity and dissolved organic matter can be different in each layer. The dispersivity is a difficult parameter to estimate but it is essentially the scale of heterogeneities in the layer. In general it is best to use a fraction of the layer thickness (e.g. 10% of the layer thickness). For thin layers such as a reactive core mat, the entire layer thickness (1 cm) might be used as a conservative approximation. Note that dispersivity is only a parameter that is relevant with an advective component such as groundwater upwelling.

Dispersivity \square 10% of layer thickness 100% of thin layers (e.g. 1 cm)

The tortuosity correction also appears in the layer definition. This is the ratio of the flow length to the straight line length through the layer and two models are recommended. The Boudreau model is recommended for consolidated materials such as sediment and the Millington and Quirk is recommended for granular materials like sand. Either can be selected by editing a particular layer and clicking on the appropriate push button.

System Properties (advection, bioturbation and consolidation)

The example system is assumed to have neither advection flow nor consolidation of the underlying sediment. You can click on System parameters to select an upwelling (positive) or downwelling (negative) groundwater flow or oscillating (tidal) flow. Both can be selected for a flow with a mean and oscillatory component. The oscillatory flow is specified by selecting a maximum amplitude and a period. **Note that the input flow velocity is the Darcy velocity in the sediment resulting from tidal or other oscillations, not the tide itself.** If the tidal amplitude is 1-2 ft, this may result in a flow amplitude in the sediment of 1-2 cm or less depending upon the permeability of the sediments. For example, we have measured an oscillation of approximately 1 cm/day (365 cm/yr) in surficial fine-grained sediments due to a tidal amplitude of 1 ft in the Anacostia River in Washington DC. In a coastal area, there are typically two tidal cycles every 24 hours 50 minutes so the period would be 0.0014 years. Other oscillating flows such as periodic flood events can be simulated by using a longer "tidal" period.

For oscillating groundwater upwelling, model output can be either instantaneous values (flux or concentration) or values averaged over the period of oscillation. This option is selected from solver options (below). Average would be the preferred choice for simulation periods that are much longer than the oscillation period. Instantaneous would only be of interest when evaluating the variations through an oscillation cycle (for example, an annual simulation with seasonal variations in flow).

Other options include the depth or intensity of bioturbation and whether consolidation will occur. A uniform bioturbation over a fixed depth can be employed or a depth dependent bioturbation where the intensity is assumed to drop off a Gaussian distribution with input standard deviation in depth. Typical values of bioturbation are a depth of 5-15 cm and intensity of particle reworking of 1-100 cm²/yr. [3]

summarized literature reported values of bioturbation depth and intensity and indicated an average bioturbation depth of 5.3 cm and intensity of $3.9 \text{ cm}^2/\text{yr}$ in freshwater systems and 12.3 cm and $125 \text{ cm}^2/\text{yr}$, respectively, in estuarine systems. Note that the depth is associated with the active layer thickness where there is active particle reworking. Isolated deeper interactions from individual organisms may occur but the areal average intensity may not be significant. Organisms also pump water back and forth but the magnitude of this value is more uncertain and is typically not important if you have a strongly sediment sorbed contaminant.

Consolidation results in an effective upwelling velocity due to porewater expression and is modeled by a maximum depth of consolidation and time scale. For example, a cap may lead to 6 in (15 cm) of consolidation with 90% of occurring in the first year. The inputs would then be 15 cm and 1 year.

Auxiliary Conditions (boundary and initial conditions)

The boundary and initial conditions (concentrations or fluxes) is set with the auxiliary condition button and conditions are set for each layer. Concentration profiles within a layer can be linear or a constant. More complicated initial concentration profiles can be set up by adding additional layers. In the example, there is an initial concentration in the porewater for phenanthrene in the sediment layer and for mercury there is an initial solid concentration.

When providing initial or boundary concentration data, the truly dissolved porewater concentration (typically that measured by passive partitioning samplers) which defines thermodynamic partitioning is expected as input. This concentration can also be estimated by the ratio of the solid concentration divided by the organic carbon based partition coefficient and fraction organic carbon for a hydrophobic organic compound. If there is significant dissolved organic carbon (DOC) or other suspended complexes, the DOC concentration and the dissolved organic carbon partition coefficient, K_{DOC} , can be input or estimated using the built-in estimates. Often the available concentration might be the result of extraction of porewater (either directly or centrifugation) and the total contaminant concentration rather than the truly dissolved concentration might be measured. In this case the input concentration should be the measured total porewater concentration and the DOC concentration should be set to 0 (since it is already included in the measured contaminant concentration).

Special consideration should be given to the surface boundary condition and the bottom boundary condition. If the surface boundary condition is set to 0 concentration, then breakthrough of contaminant might never be observed since the concentration at the surface is always forced to be 0. A better condition might be to employ a mass transfer boundary condition at the surface with the overlying water concentration. **The mass transfer coefficient can be estimated using the characteristics of the overlying water and is typically of the order of 1 cm/hr . Note, however, that the surface mass transfer may not control the rate of migration from the sediment and so this may simply be equivalent to setting a 0 concentration at the surface. If it is desired to clearly see migration of contaminants to the surface it may be best to artificially set a mass transfer coefficient to a very low value which effectively means that there is no release from the sediment surface and the concentration at the surface will increase as the contaminant migrates from below.**

A final option for surface boundary condition is a finite mixed water column. The key parameter for this condition is a residence time in the waterbody. Clicking on that option brings up a menu that allows a user to input water volumetric flow, waterbody volume, depth, DOC concentration and evaporation rate and contaminant degradation rate. The boundary condition uses the flux from the sediment-water

interface to estimate the quasi steady state water column concentration with these parameters. The boundary condition assumes that the finite water column responds immediately to any changes in flux from the sediment.

The bottom boundary is normally set at the bottom of a contaminated sediment layer. The most common conditions would be to set this layer at a measured deep sediment porewater concentration (if known) or at the concentration of the sediment layer above it (if not known). The flux matching condition could also be used at the bottom boundary. If the modeled sediment layer is sufficiently deep, these conditions will have little effect on the modeled solution.

Simulation Conditions (run duration and numerical discretization)

Solver options allow the user to set the simulation duration in the time units that were selected as well as whether average or instantaneous outputs are requested (in the oscillating flow case). This option also allows the user to set discretization and numerical solver options. The default options are very stable and likely to lead to a result with minimal numerical errors. It may, however, require a long time to run in some simulations, particularly with a combination of thin and thick layers, rapid tidal oscillations, multiple species and reaction and nonlinear sorption or reaction. The model run times can be shortened by use of manually defined discretization options but note that model instability may result. The fastest solutions to generate are those that are run with a uniform number of grid cells in each layer and use of the fastest layer to set the time step. If you have a multi-core processor you can also run multiple independent simulations at the same time since PYTHON is not designed to effectively use multi-core processors.

The model run time can often be shortened dramatically by choosing different simulation parameters. In general you can select "User-defined" time and spatial steps using larger time steps and larger spatial grid size (fewer spatial grid points). Note that when oscillating flows are selected, the model will reset the time step as necessary to require at least four time steps per oscillation period. This can lead to longer time requirements if you have a short period oscillation (e.g. tides) that you are trying to simulate. If you are concerned about the accuracy or stability of your solution, you can then decrease the time step and increase the number of spatial grid points and make sure that this does not appreciably change your solution.

You can also change the time required by employing an implicit method versus the Crank-Nicolson method. You might also employ the implicit method if you see some instability or oscillations in the Crank-Nicolson solution.

File Options and Execution

The final input screen is the "Edit File Options" button and this allows you to name files. By default the name is not changed and your results will write over your previous results unless you change the name. The completion of inputs is noted by pushing the Ok button and then run simulation. The example application will take approximately 5 minutes to run as a result of the multiple coupled reactions.

Output

The completion of model execution leads to an output which by default is the concentration profile of the first contaminant as a function of position at different times. In the example simulation case, phenanthrene is showing depletion from the surface of the sediment over time and migration into the overlying layers. The y axis extends to -5 cm after 50 years due to the deposition of 0.1 cm/yr in this problem. The plotted concentration is the freely available (or truly dissolved) concentration if that were

what was input in the auxiliary condition tab. You can also show “Total Concentration” which is the sum of the truly dissolved and colloidal organic carbon bound contaminant concentration as well. Note that if you used a total concentration as the contaminant concentration in the auxiliary conditions and set the dissolved organic carbon to 0, the concentration is already the total concentration. **Note that there is a subtle difference between these two cases. If you input truly dissolved concentration and the dissolved organic carbon in each layer, the dissolved organic carbon is not assumed to diffuse but remains as defined in each layer (but any advection will transport both DOC associated and truly dissolved contaminant). DOC molecules are relatively large and typically have much lower diffusion coefficients than a dissolved contaminant. If you input total concentration and set DOC =0, however, the DOC associated contaminant is assumed to diffuse just as if it were the dissolved contaminant (as well as be transported by advection).**

When you plot time profiles, you have the option of plotting 0 relative to the initial sediment-water interface or the sediment-water interface at any time. Click “Edit plot” and choose “Time profile” and “New benthic surface” and depth of interest of 0. If you wish to see concentration within the surface layer, choose the middle of the bioturbation layer (e.g., 2.5 cm in a 5 cm bioturbation layer). The result is a relatively smooth prediction of the concentration in the middle of the biologically active zone that doesn’t reflect the oscillations at the surface.

You can also view other plots if desired. You can push the button “Edit plot” and select the desired spatial or time plots for porewater concentrations, fluxes, total concentrations and solid concentrations in various solid materials. You can change the size, legend location and axis limits by using the “Edit Figure”. In the same window, you can choose ‘Show sketch’ to add 2-D column spatial-temporal sketch on the left beside the plotting graph as a brief for the simulation system.

If you see things that you wish to change in the simulation, push “Modify System”. If you are happy with the simulation, you should export the result and a popup window will allow you to choose a name and location. In general use the default location which is the output subdirectory in the CapSim directory. This data can be brought back to the same plot and compared to other files using the Main Menu option “Load Existing Results”. The plot options are the same as in the output screen except you can import multiple result files and plot them all together.

Advanced Topics

Problems with using $z=0$ for output

As noted previously, $z=0$, the values calculated for $z=0$ may reflect the boundary condition at the surface more so than migration from below. Thus concentration migration from below would not be obvious if the concentration is forced to 0 at the top. A better option would be to evaluate the flux or concentration at a layer deeper into the sediment, e.g. the middle of the biologically active zone. You could also change the boundary condition at the surface so that you could see migration from below, e.g. by setting the mass transfer coefficient very low so that contaminant would accumulate at the surface if migrating from below.

Deposition will also affect the concentration at the surface. Deposition in CapSim is modeled by adding a new grid cell when sufficient deposition has occurred. Thus deposition will result in fluctuations over time

as grid cells are added. In the example case, we can change “Depth of interest” value on the figure to measure how concentration and flux vary versus time with a specific depth below initial benthic surface. The default value 0 means the initial benthic surface. Because of bioturbation, the concentration and flux of phenanthrene versus time curve will fluctuate between 35yr to 40yr in this example. If we select “new benthic surface”, it shows the concentration and flux variation on the current benthic surface that is steadily moving up due to deposition.

Sorption kinetics

Sorption can be modeled as a local equilibrium process or as a kinetically limited process. This may be particularly important for strongly sorbing media such as activated carbon and strongly hydrophobic contaminants such as PCBs. Kinetic sorption is selected by editing sorption properties and choosing the equilibrium/transient pushbutton. A kinetic rate coefficient can then be entered or by pushing the Kinetic rate coefficient? button, a half-life can be entered and a rate coefficient calculated. Sorption is modeled as first order so the first order rate is simply a first order rate constant regardless of sorption isotherm used. The desorption rate is modeled as linear or nonlinear to ensure consistency with the selected isotherm.

Sorption kinetics is of concern when the time scale for kinetics, $\tau_{sorption} \sim 1/k_{sorption}$, is of the same order or longer than the residence time in the sorbing layer. The residence time, τ_{res} , can be estimated by

$$\tau_{res} = \frac{1}{1/\tau_{diff} + 1/\tau_{adv}} = \frac{1}{16D/h^2 + U/h} = \frac{h^2}{16D + Uh}$$

Where U is the Darcy velocity in the layer, D is the effective diffusion/dispersion coefficient and h is the layer thickness. Sorption kinetics have a significant impact on migration through the layer when $\tau_{sorption}/\tau_{res} \geq 0.2$. At $\tau_{sorption}/\tau_{res} \geq 1$, a contaminant will migrate in a layer approximately twice as fast as a contaminant that would be in local equilibrium.

A user is also cautioned that if sorption kinetics are considered, a smaller time step may be needed for the simulations. One indication of this may be simulations with kinetics that seem to fail, that is they do not complete. In such cases, a simulation should be aborted and a smaller time step selected. This would normally be for situations where fast sorption kinetics is simulated so it may also be possible to assume equilibrium rather than trying to simulate fast sorption kinetics.

Reactions

The default model for reaction is first order, you can choose “user-defined” and input the index value for the rate equation. For organic decay, you don’t need to worry about products.

Changing the reaction rate index value will mainly cause the variation of concentration and flux of the specific chemical and probably have little influence on the other chemicals. But by increasing the index value, the system’s non-linear properties will be increased, which will decrease the stability.

You can also input multiple compounds that are linked through reactions and products. The more complicated the reaction network, however, the slower the model simulation and potentially the greater the likelihood increased instability. CapSim is probably best used for relatively simple reaction networks

for no more than 3-5 reactants and products that are linked. In principle, however, there are no limits on the complexity of the problem you wish to solve.

Fast reactions may also cause the same phenomena as indicated for fast sorption processes. That is, a smaller time step may be required than would otherwise be the case.

Effect of deposition and oscillating velocities

After increasing the deposition velocity, the grid numbers will automatically change back to defaults, so you may need to change it. If the system being simulated is a complicated non-linear system, increasing deposition velocity will increase the system's instability, which could lead to a failure to achieve convergence to a solution. You can modify the grid number and time step to decrease the instability of the system. Deposition is modeled by adding a grid when sufficient deposition has occurred to do so. This leads to some oscillations although the model output is automatically averaged so they may not be important.

By increasing oscillating velocity, the calculation time will increase and the flux versus time curve will fluctuate more obviously if the instantaneous option is selected. This does not, however, mean that the system is unstable. It may simply be tracking the fluctuations that are actually occurring in the system.

Note that a high frequency fluctuation (e.g. twice per day tidal fluctuations) may not be synchronized with your output file (e.g. 1000 output values for example means that the output times saved are 1/1000 of the total simulation time). In such cases, the output may catch different parts of the fluctuation cycle and show fluctuations that do not accurately capture the frequency or amplitude of the fluctuations. If capturing the fluctuations are desired, the values should be output at a greater frequency than the actual fluctuations.

$$\text{Frequency of output} > \text{Frequency of fluctuations desired to track}$$

In general, for simulation times that are long relative to the oscillation period, the averaging option should be selected in the solver options.

Unstable solutions

According to the central differencing scheme, maximum Pe number should be less than 2 in case of overcoming instability, but the system is designed to modify Pe automatically so users don't need to worry about this. If users observe unstable model results (i.e. oscillating solutions or solutions that "blow up") for a non-linear system (including Langmuir sorption or Freundlich sorption), decreasing time step is the most useful method to try, at the same time, they can also increase grid number to shorten grid size and let the system have more points to do the calculation for non-linear system. Switching to the implicit method for solution can also be helpful.

As indicated above, too large a time step may also lead to a failure for nonlinear simulations to converge and the system seems to "hang". In such cases, the first step is again to abort the simulation and reduce the time step.

Speeding up CapSim for Complex problems

Sometimes, CapSim will take several thousand seconds to finish the simulation. To speed up CapSim for complex problems, we can decrease the grid number and thus enlarge the grid size, and at the same time, we can increase time step and lower the simulation duration to shorten the calculation time. There is a lot of flexibility in CapSim to speed up the simulation. It is always a good idea to test a complicated simulation by ensuring that decreasing the time step and decreasing the spatial grid size does not appreciably change the results. If that is the case, you can use the larger time step and spatial grid to routinely solve the problem.

1. Thoma, G.J., Danny D. Reible, Kalliat T. Valsaraj, and Louis J. Thibodeaux, *Efficiency of Capping Contaminated Bed Sediments in Situ 2. Mathematics of Diffusion-Adsorption in the Capping Layer*. Environ. Sci. Technol., 1993. **27**(12): p. 2412-2419.
2. Palermo, M., et al., *Guidance for in situ subaqueous capping of contaminated sediments*. EPA 9056B966004, 1998.
3. Reible, D.D., *Sediment and Contaminant Processes*, in *Processes, Assessment and Remediation of Contaminated Sediments*. 2014, Springer. p. 13-24.